



Science Gateway for Cyber and Software Automation in Neuroscience

Prasad Calyam, PhD
Associate Professor,
Department of Electrical Engineering & Computer Science

(Collaborator: Prof. Satish Nair)

Gateways 2018

“VIMAN Lab” Cloud Computing Research

<http://faculty.missouri.edu/calyamp>



VIMAN Lab

VIRTUALIZATION, MULTIMEDIA AND NETWORKING LAB

- Cloud Resource Allocation
 - Computer and network virtualization models, algorithms, tools
- Cloud Monitoring
 - Software-defined measurements and performance diagnosis
- Cloud Testbeds for Apps, Marketplaces
 - e.g., Manufacturing/Healthcare/Education/Public Safety
- Cloud Security
 - Cyber attacks defense, Federated Resource Policy Management



Science Gateway to Accelerate Neuro Big Data Research & Training

- **Big Data has to be “social” – addressing a crisis!**

CyNeuro goal is to spur computational and cyber neuro research at Mizzou and collaborator institutions via: (i) the development of ‘free’ cyber and software big data tools for neuroscience research, and (ii) facilitation of interactions among physical sciences faculty with big data expertise (engineering, math, statistics, physics) and wet-lab, behavioral and clinical neuro faculty with big data ‘needs’.



This project is supported partly by the National Science Foundation under the award number OAC-1730655

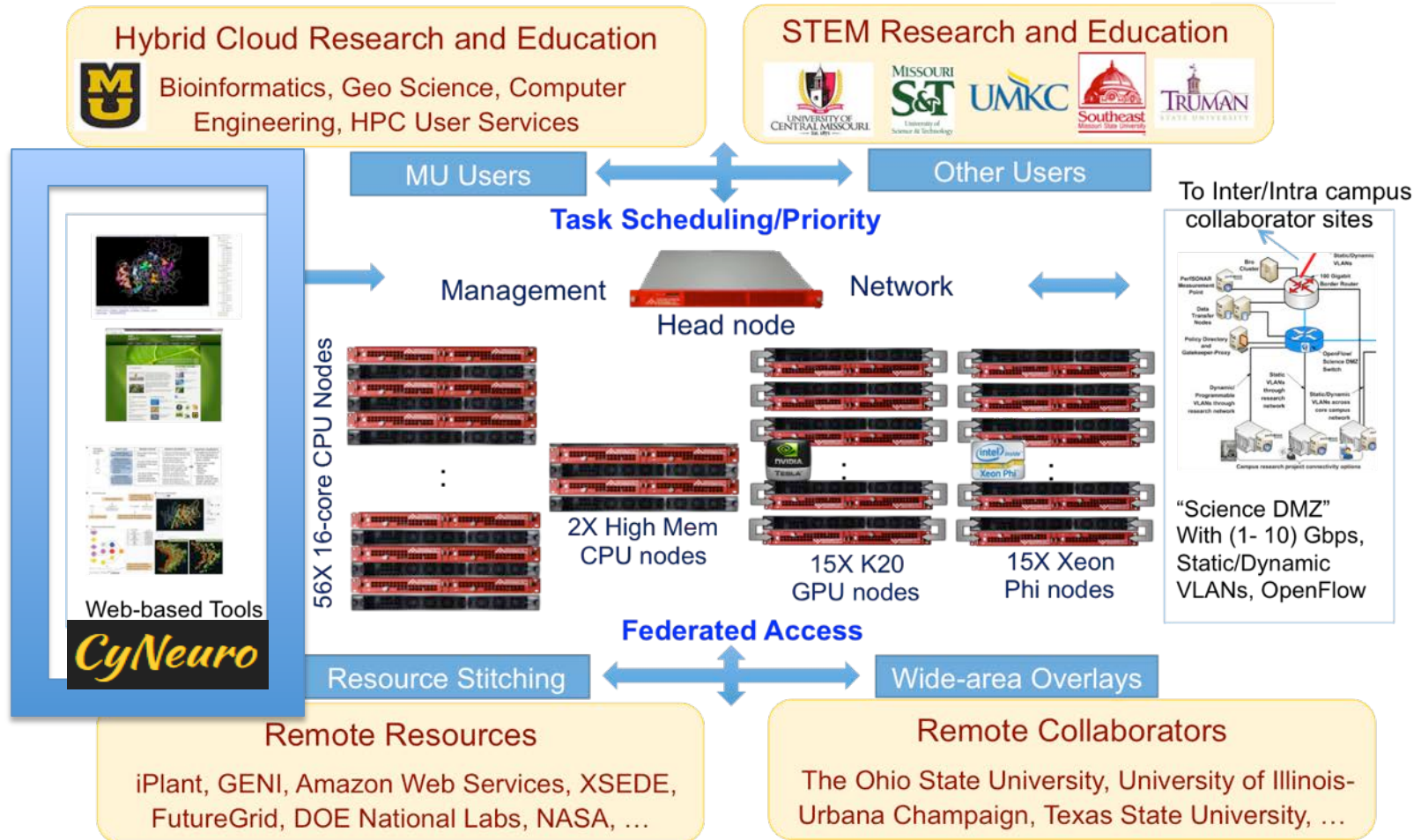
Big Data Researcher Journey...

- ① **“I have observed an interesting phenomenon, is this really interesting to create a research goal/hypothesis?”**
 - What additional data exists?
 - Whose expertise can I leverage?
 - Where can I get the necessary storage and computation?

- ② **“I have a working sandbox, but how can I scale up?”**
 - Are there tools to automate/visualize/Debug my workflows?
 - How can I build/join a ‘community’ around my Big Data?
 - What cyberinfrastructure do I need to move/analyze Big Data?

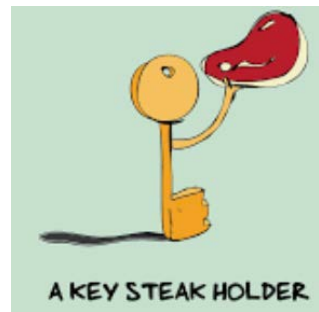
Cloud Vision for MU Cyberinfrastructure

(Supported by NSF CC-NIE & NSF MRI/CCIIIE)
(Leads: Dr. Calyam, Dr. Shyu, Dr. Springer, Dr. Xu)



MU is building a **Big Data eco-system** for science and engineering research and education – features advanced cyberinfrastructure technologies

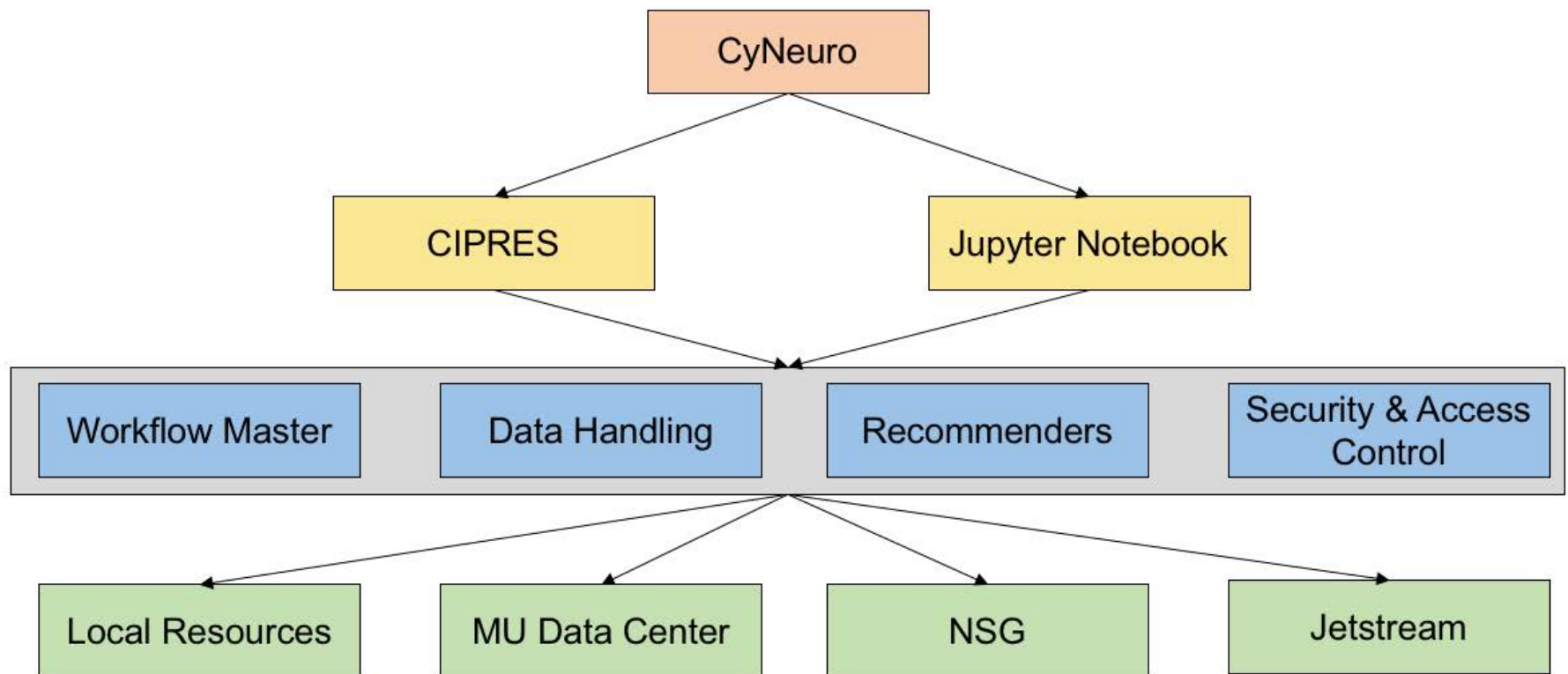
CyNeuro is



of



- Thank you Mona Wong @ SDSC!



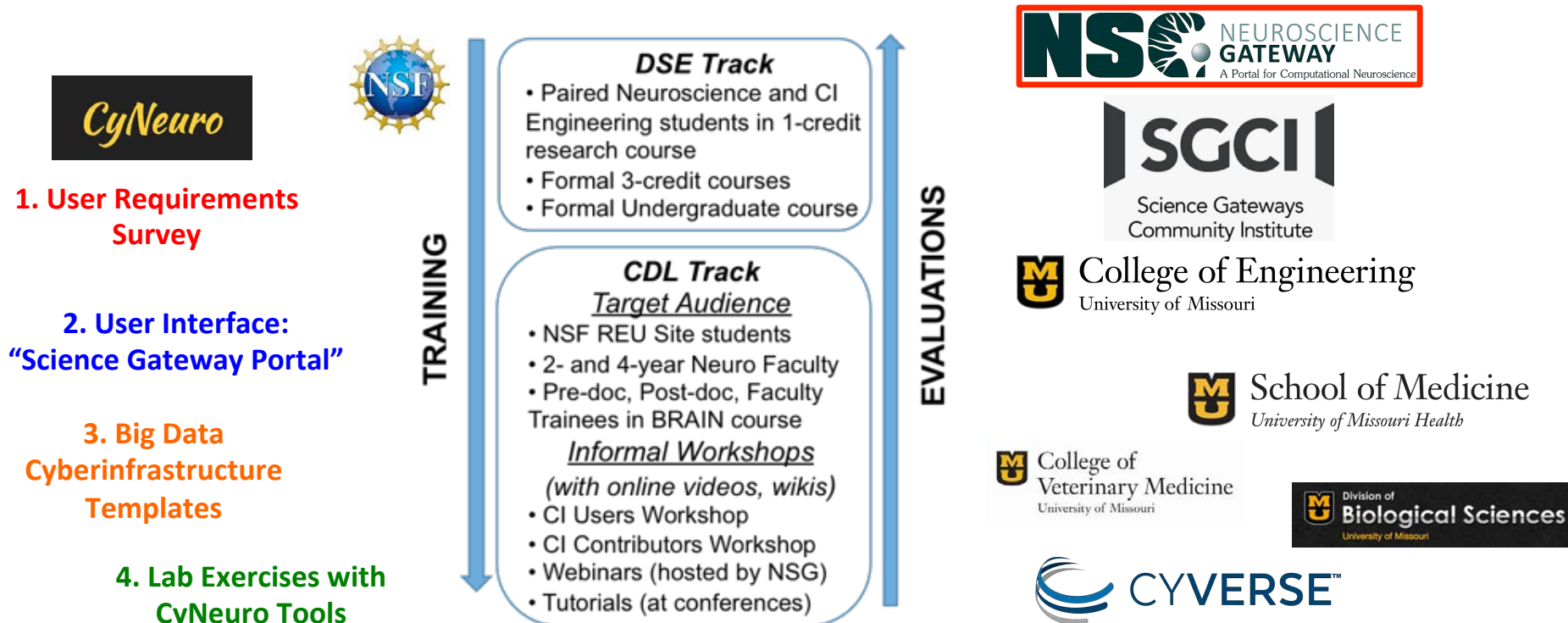
Fostering Neuroscience Big Data Training & Research across MU

(Supported by NSF CyberTaining; Leads: Dr. Nair, Dr. Calyam,

Collaborators: Dr. Xu, Dr. Ho, Dr. Joshi)

- “Research on training” of software & cyber automation tools in neuroscience to address the emerging needs involving big data

Students use cutting-edge cloud resources in MU cyberinfrastructure, CyVerse & Neuroscience Gateway



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MU » Engineering » Computational Neurobiology Center » **Training & Outreach**

Training & Outreach

The Nair Lab coordinates the following training and outreach activities



GRADUATE RESEARCH TRAINING.... for Pre-docs, post-docs, Medical Students, Residents and Research FACULTY from all interested disciplines

[NIH BRAIN Initiative Summer Course \(2016-2018\)](#)

UNDERGRADUATE RESEARCH TRAINING.... for undergraduate students (from outside Missouri) from all interested disciplines (biology, engineering, psychology, physics, mathematics,...)

[NSF Research Experiences for Undergraduates in Computational Neuroscience \(2017-2019\)](#)

FACULTY TEACHING for faculty (and high school teachers) from Biology, Psychology, Engineering, Physics, Math,...interested in teaching undergraduate neuroscience

[NSF Summer Neuroscience Workshop](#)

since 2007 (Impact: **113 biology and psychology undergraduate faculty from 27 US states)*

K-12 for Science and Math teachers are all levels

[Elementary Engineering Academy](#)

Middle School Neural Engineering coming soon

High School Neural Engineering coming soon

ECE 8001 Course

“Software and Cyber Automation in Neuroscience”

- 1-credit ***project-only*** course offered in **Fall 2017, Spring 2018**
 - 10+ students from Nair Lab, Calyam Lab, Xu/Joshi Lab
 - Project activities need to bridge the knowledge gaps at the national-scale (e.g., NSG, CyVerse) and MU campus (our CyNeuro)
- Fall 2017 Course Deliverables for Students
 - **In-class presentations** – each group given 3 presentation opportunities to **share progress on the 4 course thrusts**
 - **Project Poster** for 1st Neuro-BigData Symposium – early October
 - **Mid-term exam**: Interim Report, Presentation, Demo of software/data/CI – end of October
 - **Final exam**: Completed Report, Presentation, Demo of software/data/CI – end of November
 - **Talk and Demo** at 2nd Neuro-BigData Symposium – mid December

Course Syllabus

(Still evolving...)

- The project(s) will focus on the investigation and development of cyberinfrastructure tools in neuroscience to address emerging needs of big data in neuroscience; example projects include:
 - Work on collecting molecular data, brain imaging, synapses, fMRI and other related neuroscience datasets and putting them together under one web resource for neuroinformatics applications
 - Compare cyberinfrastructure resource allocation technologies and policies in MU, CyVerse and Neuroscience Gateway
 - Integrate multiple cyberinfrastructure tools such NEURON (<http://www.neuron.yale.edu>) and VCell Virtual Cell (<http://vcell.org>) into one pipeline for complex neural simulations
 - Build high performance computing and cloud based workflows and algorithm optimization as suitable for diverse analytics from distributed data sources

1. User Requirements Survey

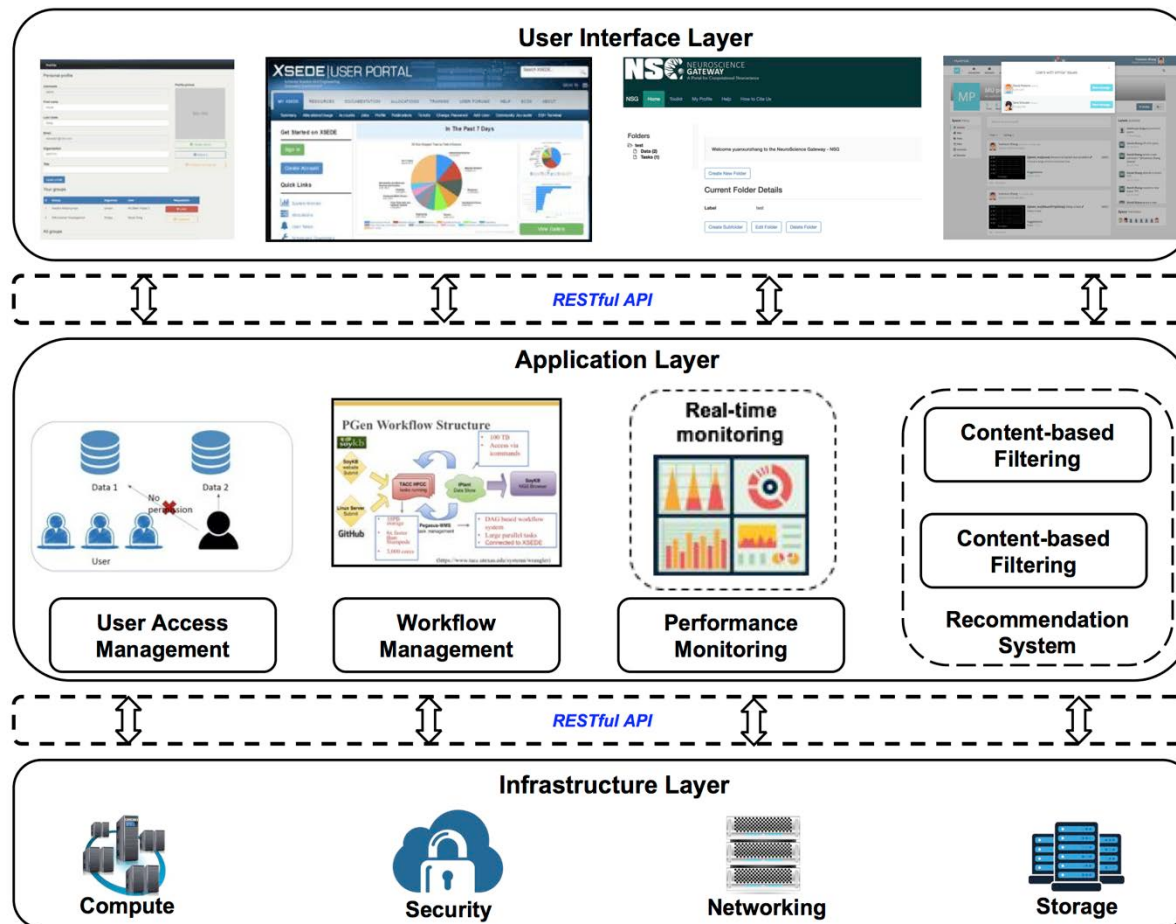
- Use cases (compute/data intensive) identified through user survey at MU
 - Use Case 1: Neural Simulations
 - Single cell modeling
 - Network modeling
 - Use Case 2: Zebra Fish Imaging
 - Use Case 3: fMRI
 - Use Case 4: WGCNA
 - Use Case 5: 2-Photon Calcium Imaging
- Online survey & 1-1 Meetings with many researchers/stakeholders
 - **Ilker Ozden, Rohit Manchanda, David Beversdorf, Mahesh Thakkar, Drew Headley**
 - **David Schulz, John Cannon, Lincoln Sheets, Pradeep Bollu, Ravi Nistala, Carmen Cirstea, ...**
 - *Issues: Data format, Database, Data Analysis, Automation, Knowledge Sharing, ...*
- Survey for users to provide requirements -
https://missouri.qualtrics.com/jfe/form/SV_5cfSAgrbYmkU2Cp

CyNeuro Gateway User Needs Summary

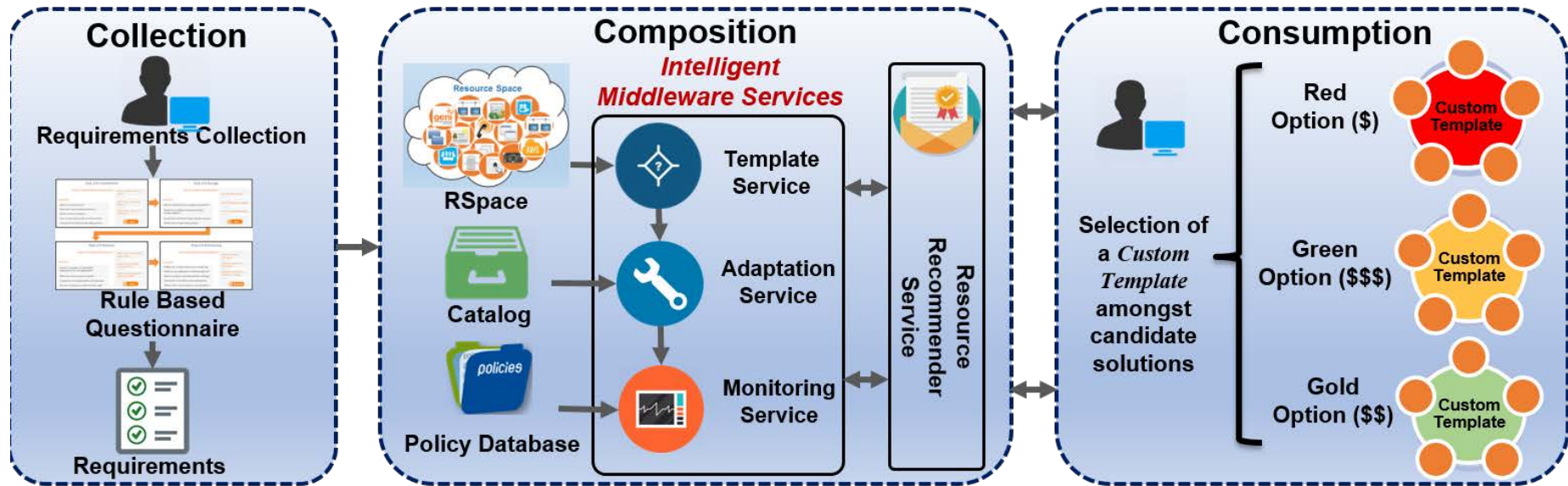
- Reproducible computing environment with easy learning curve
- Easily customize the pipelines and ability to re-run analyses on the same data
- Quick data processing (using local or remote resources)
- Entire analysis should be easy - setting up an experiment and collecting data
- Compelling visualizations to share with scientific community
- General purpose tutorials with documentation

2. User Interface: CyNeuro Gateway

- We aim to define and develop a “**Neuro BigData Science Gateway**”
 - Motivations from SoyKB, CyVerse, NSG, ...



3. CyNeuro Templates



Custom Template Lifecycle

- Catalog with pre-defined templates for workflows to help novice users
- Users can either customize the existing templates or create their own templates, which will be stored in a “Catalog”
- Storing templates in a **Catalog will help to “reuse” or “repurpose” of workflows**



CyNeuro

BROWSE ▾

ANALYTICS ▾

EVENT ▾

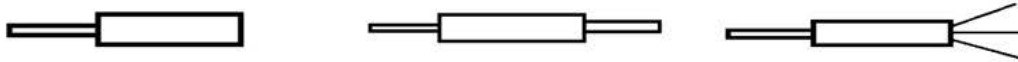
ABOUT ▾

👤 Introduction

♥ Create Workflow

✉ Monitor Workflow

SINGLE NEURON WORKFLOW REQUIREMENTS



Workflow Automation & Management

Soma length		?
Soma Diameter :		?
Dendri length:		?
Axon length:		?

Back

Next

EXPERT AGENT

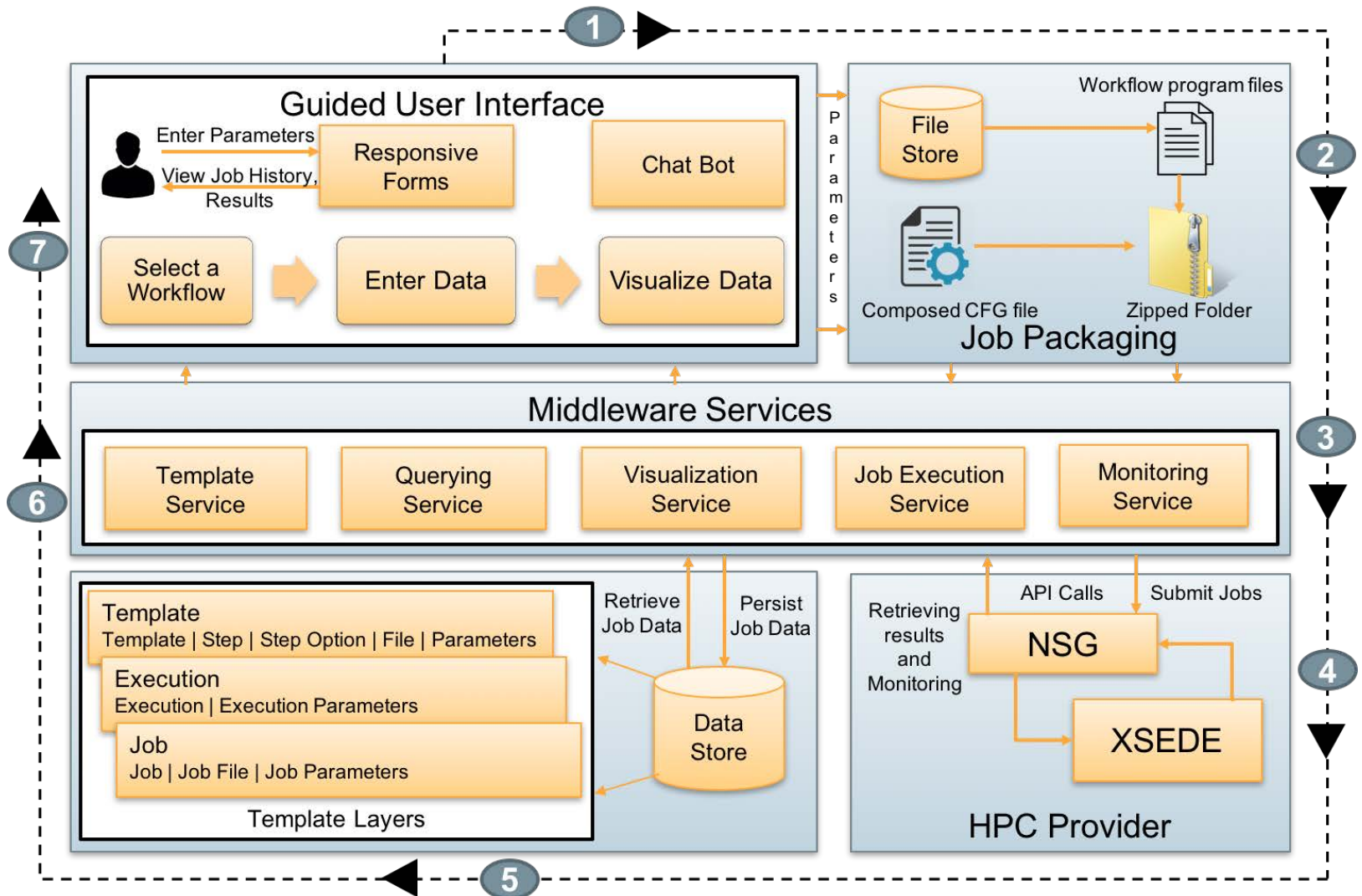


VIMAN : 1) Collecting length
Collecting Soma length &
diameter.
Collecting Dendri length
2) Choose Channels
Selecting Sodium, Potassium
and Calcium.
3) Choosing Voltage and
Current
Membrane voltage and current.

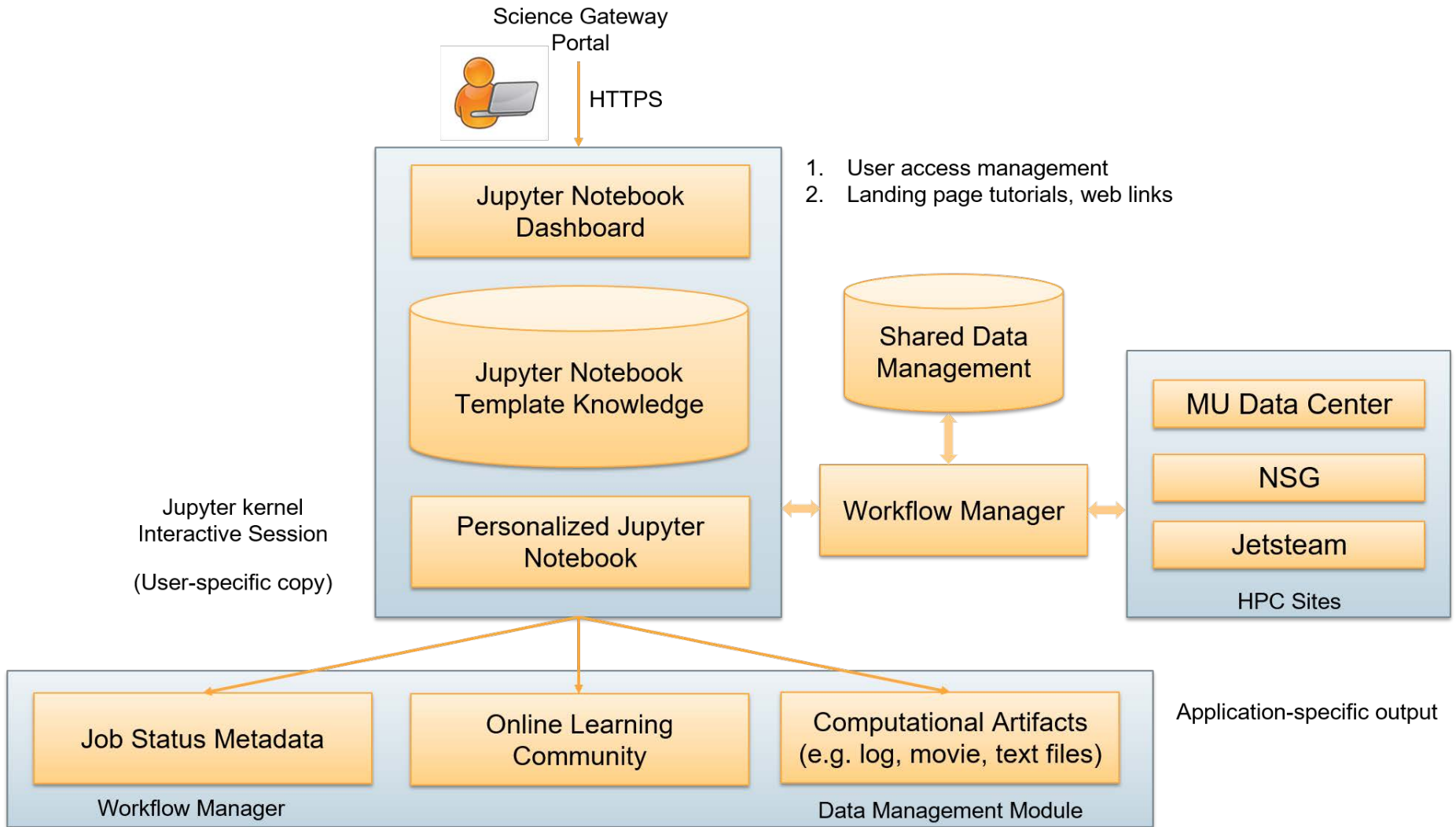
Do you want to run a simple
single experiment?

CyNeuro Portal v1

- Cyber and Software Automation Components



CyNeuro + Jupyter Notebooks



Jupyter Notebook example showing NEURON code in a passive cell tutorial

Passive Cell Tutorial

In [2]: `from neuron import h
from matplotlib import pyplot
%matplotlib inline
h.load_file('stdrun.hoc')`

Out[2]: 1.0

1) Create the cell and define its geometry

NEURON defines it as a cylinder so we only need to give length and diameter

In [3]: `#Create the soma section and define the default parameters
soma = h.Section(name='soma')
soma.diam = 200 #default is micrometers
soma.L = 100 #um`

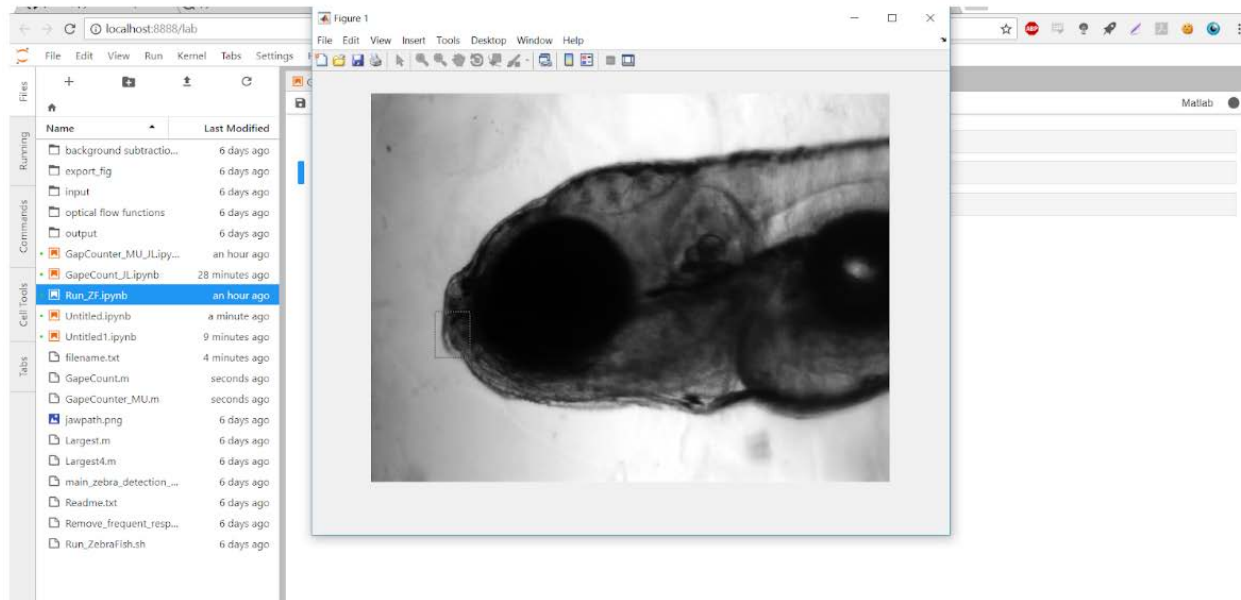
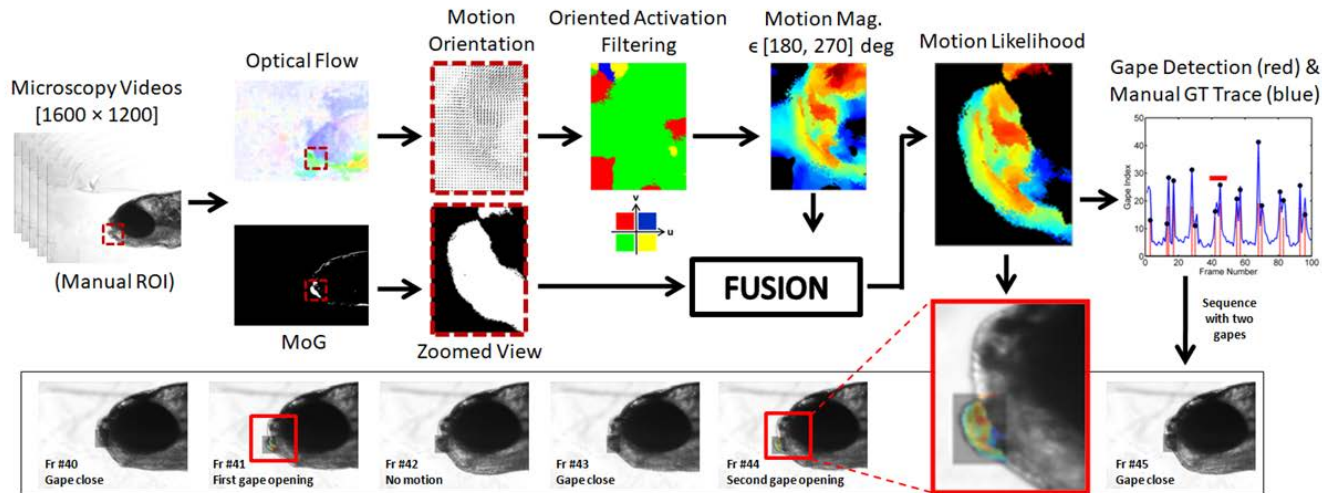
2) Define the cell's biophysics

Web-link for shared NEURON Jupyter notebook

Python-based notebook

Python 2

Jupyter notebook demonstrating the Zebrafish Use Case



CyNeuro.org

CyNeuro

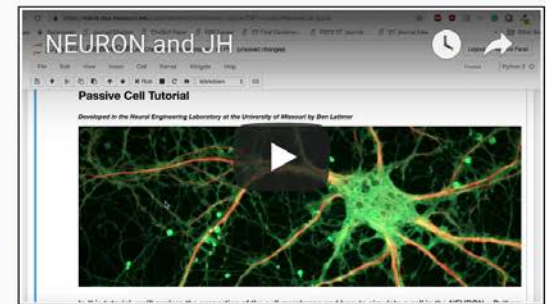
ABOUT ▾

PROJECTS ▾

EVENTS ▾

Neuron simulation using Jupyter Notebook <https://metis.dsa.missouri.edu/> New

Jupyter Notebooks are documents that contain computer code and rich-text elements (e.g., equations, figures, web links) in order to enable the user (i.e., an instructor or student) to inspect the state of an execution in real-time. This server-client application has the flexibility to edit and execute a custom notebook on a local desktop without Internet access or via web-access on a remote server. These features allow the simulations to be modified and communicated in an understandable and reproducible manner and can be used to remotely deliver instructional material to a large group of remote students.



We developed Jupyter Notebook instances for exemplary teaching and research use cases of neuroscience users. Users can use pre-built notebooks to learn how to model a neuron cell using NEURON python tool. By obfuscating the underlying Python code, the NEURON-based notebooks allows the non-programmers to focus on experimenting with the parameters for neuron simulations. This approach also enables the instructors to focus on the learning material and teaching objectives during the class, instead of addressing trivial issues such as environment configuration, credentials for software access, or other installation problems.

Note: Please email Dr. Satish Nair for accessing Jupyter Notebook server.

NSG-R Jupyter Notebook Coming soon

Pre-configured Jupyter notebooks for submitting neuron jobs to NSG. Users can use this notebook to submit modeling and simulation jobs. Researchers who are familiar with neuron job submission can use these notebooks to access and run

VIDEO COMING SOON

Course Users Survey

- **Course User Groups**

- Application User Team - Neuron/network simulations
- Application User Team - MATLAB-based image processing automation
- CI Engineer Team – distributed CI resource management using Lewis and NSG
- Science Gateway Portal Developer Team - Jupyter Notebooks and CIPRES configuration

- **Lessons Learned**

- Interdisciplinary project outcomes benefitted from application and CI users having regular and frequent feedback
- Prototype Demos by CI users better engaged application users
- CI students needed additional training and survey science concepts understanding for better engagement with application users

Call for Participation

NATIONAL WORKSHOPS FOR CYBER AND SOFTWARE AUTOMATION IN NEUROSCIENCE

- **Join us for a 3-day workshop in **early February 2019****
 - Theme of: “***Annual Neuroscience Cyberinfrastructure Users/Contributors Workshop***”
 - All expenses to attend the workshop will be covered through NSF-supported travel grants
 - We welcome participants to apply (including undergraduate and graduate students, PostDocs, research faculty, educators, system administrators, network engineers, and industry)



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